Journal of Computational and Applied Mathematics 31 (1990) 199–203
North-Holland

A point method for a semi-conductor equation

Joachim WICK
Fachbereich Mathematik, University of Kaiserslautern, Erwin-Schrödinger-Straße, D-6750 Kaiserslautern, FRG

Received 2 March 1989
Revised 12 November 1989

Abstract: In this paper we present a numerical method solving kinetic equations for semi-conductors. The method is based on a finite-point approximation of the initial distribution and a rediscretization of the gain term in the collision integral. This is made using sequences of uniform distribution. Also the convergence of the method is shown with this number-theoretical approach.

Keywords: Kinetic semi-conductor equation, point approximation, low-discrepancy methods.

1. Motivation of the equation

The development of semi-conductors is based on a drift-diffusion model [2], which was obviously very powerful. But such a model has a certain range of admissibility. Since the technology has improved, it becomes more inaccurate. To overcome this, one goes back to the derivation of the model. The source is an equation of Boltzmann-type

$$\left(\partial_t + v\,\partial_x + \dot{k}\,\partial_k\right) f(t, x, k) = Q_{\text{coll}}, \tag{1}$$

where $f(t, x, k)$ is the single particle density function in the position- and wave vector-space at time t. This is a one-electron approximation and closely connected with this is the bandstructure, which describes the energy $\mathscr{E}(k)$ of state k as a function of k. The equations of motion under the influence of the applied field K and the self-consistent Lorentz force are

$$\dot{x} = v(k), \qquad \dot{k} = \frac{\mathrm{e}}{\hbar}(E + v \times B + K),$$

where the group velocity of the carrier is given by

$$v(k) = \frac{1}{\hbar}\,\partial_k \mathscr{E}(k).$$

The collision term Q_{coll} describes the rate of change of f due to scattering with thermal bath via phonons and imperfections. If we neglect carrier–carrier scattering the collision term becomes linear:

$$\int_B P(k, k') f(t, x, k')\,\mathrm{d}k' - C(k) f(t, x, k),$$

where P, C are nonnegative, smooth and

$$\int_B P(k, k')\,\mathrm{d}k = C(k').$$

The integration is carried out over the first Brillouin-zone $\mathscr{B}$. E and B are the self-consistent electro-magnetic field described by Maxwell's equations.

We are searching for a solution in $(0, T) \times \Omega \times \mathscr{B}$, where

$$f(0, x, k) = f_0(x, k) \quad \text{and} \quad f(t, x, k)\,|_{x \in \partial\Omega} = g(t, x, k)$$

are given [8].

Now, it seems hopeless to solve this problem analytically. If we apply usual discretization methods as finite differences or Fourier expansions the dimensionality of the problem allows a very poor discretization only. Therefore, we have to look for other methods.

2. Motivation of the method

The left-hand side of (1) has the same structure as the Vlasov equation in plasma physics

$$\left(\partial_t + v\,\partial_x + \frac{\mathrm{e}}{m}(E + v \times B)\,\partial_v\right) g(t, x, v) = 0,$$

where g describes the phase space density of electrons. E and B are again the self-consistent electro-magnetic field described by Maxwell's equation. For this Vlasov–Maxwell system the finite-point approximation is well established. There are codes for the full 3D-problem since 1982 [1], and we have also a mathematical justification of the method [6,7]. Hence it is reasonable to extend this technique to this problem.

A finite-point approximation of the Vlasov–Maxwell system can be described in terms of discrete measures, and the Vlasov dynamics preserves a discrete measure

$$f(n\,\Delta t, x, v)\,\mathrm{d}x\,\mathrm{d}v \approx \mu_N^n := \frac{1}{N}\sum_{i=1}^{N} \delta(x - x_i^n)\delta(v - v_i^n)$$

and

$$v_i^{n+1} = v_i^n + \Delta t \frac{\mathrm{e}}{m}(E + v_i^n \times B), \qquad x_i^{n+1} = x_i^n + \Delta t\, v_i^{n+1}. \tag{2}$$

To transfer this to the semi-conductor case, (2) defines an intermediate measure $\tilde{\mu}_N^{n+1}$, replace v by k and add the external field K to the Lorentz force. Then we calculate

$$\hat{\mu}_N^{n+1} := \tilde{\mu}_N^{n+1} + \Delta t\left(\int P(k, k')\tilde{\mu}_N^{n+1}(\mathrm{d}k') - C(k)\tilde{\mu}_N^{n+1}\right). \tag{3}$$

Unfortunately, this is a mixture of a discrete and an absolutely continuous measure. And the absolutely continuous part is unavoidable from the structure of the gain term

$$\int P(k, k')f(t, x, k')\,\mathrm{d}k'.$$

If we substitute $\tilde{\mu}_N^{n+1}$ by $N^{-1}\Sigma\int\omega_1(x - x_i^{n+1})\omega_2(k - k_i^{n+1})\tilde{\mu}_N^{n+1}$ $(\mathrm{d}k, \mathrm{d}x)$ in (3), where ω_i, $i = 1$, 2, are mollifiers, the result is an absolutely continuous measure. In principle, this can be approximated by a discrete one, but until now no fast algorithm is available.

For another approach we remark that for the solution of Maxwell's equation the charge density must be computed. This is done by introducing a grid in the space region Ω and by distributing the point charges among the grid points. For this purpose several sophisticated techniques are developed. Since a collision is a local process we try to adapt these techniques also for the computation of the collision integral. However, Moock [3] has shown that only the nearest grid point approximation (NGP) leads to a convergent approximation. This means, all particles in one cell count in this cell only.

For that reason and since (2) is well understood we can concentrate ourself on the approximation of the collision integral for a fixed space coordinate. This means, we study the simple equation

$$\partial_t f = \int P(k, k') f(t, k') \, dk' - C(k) f(t, k) \tag{4}$$

and for a first attempt we reduce the dimension to $n = 1$. For simplicity we normalize the range of integration to [0, 1].

3. Convergence result

We define

$$\frac{2i-1}{2N} = \int_0^{k_i^{n+1}} \hat{\mu}_N^{n+1}, \quad i = 1, \ldots, N, \quad \text{and} \quad \mu_N^{n+1} := \frac{1}{N} \sum_{i=1}^{N} \delta\left(k - k_i^{n+1}\right).$$

Using number-theoretical results, we can show the next theorem.

Theorem 1 (Motta et al. [4]). *Let f be the solution of* (4), $f(0, k) = f_0(k) \geqslant 0$; $\int_0^1 f_0 \, dk = 1$ *and* $\int_0^1 P(k, k') \, dk = C(k') = \text{const}$. *Then μ_N^n defined above converges weakly to μ_t as $N \to \infty$, $n \, \Delta t \to t$,*

$$\mu_t(dk) = f(t, k) \, dk \quad \textit{and} \quad N \Delta t \to \infty.$$

Corollary 2. *The theorem remains true, if the range of integration in* (4) *is extended to the whole axis, provided for the solution holds additionally*

$$f(t, v) = O(v^{-2}), \quad |v| \to \infty.$$

Proof. We consider the transformation

$$k := \frac{v}{2(1 + |v|)} + \frac{1}{2}.$$

Then

$$v = \frac{2k-1}{1 - |2k-1|}, \quad \frac{dv}{dk} = \frac{2}{(1 - |2k-1|)^2}, \quad k \in (0, 1),$$

and it is easy to see that the function

$$g(t, k) := f\Big(t, \frac{2k-1}{1-|2k-1|}\Big) \cdot \frac{2}{(1-|2k-1|)^2}$$

fulfils the requirements of the theorem. □

4. Numerical results

Here we consider the master equation in kinetic theory, which has the same structure as (4):

$$\partial_t f = \int_{-\infty}^{\infty} \exp\big(-(v-v')^2\big)\big(f(t, v') - f(t, v)\big)\, \mathrm{d}v', \tag{5}$$

$$f(0, v) = \frac{1}{\sqrt{2\pi}} \exp(-v^2).$$

The advantage is that the exact solution can be computed too. This example is also solved by Nanbu [5] in a Monte Carlo simulation technique. He uses 10 000 particles and performs 10 runs for an averaging. We get the same accuracy using 2047 points, but for less points we observe strange oscillations in the results.

They vanish, if we modify our scheme as follows:

$$\eta_0^{n+1} = -\infty, \qquad \frac{i}{N} = \int_{-\infty}^{\eta_i^{n+1}} \hat{\mu}_N^{n+1}, \quad i = 1, \ldots, N-1, \qquad \eta_n^{n+1} = \infty,$$

and define

$$\bar{v}_i^{n+1} = \int_{\eta_{i-1}^{n+1}}^{\eta_i^{n+1}} v \hat{\mu}_N^{n+1}(\mathrm{d}v), \quad i = 1, \ldots, N, \qquad \mu_N^{n+1} := \frac{1}{N} \sum_{i=1}^{N} \delta\big(v - \bar{v}_i^{n+1}\big).$$

Then the convergence theorem is still true.

To understand this, we perform another approach. We can write the equation (5) in divergence form:

$$\partial_t g - \partial_v G = 0, \qquad G(t, v) := \int_{-\infty}^{v} \int_{-\infty}^{\infty} \exp\big((\tilde{v}-v')^2\big)\big(g(t, v') - g(t, \tilde{v})\big)\, \mathrm{d}v'\, \mathrm{d}\tilde{v},$$

and consider the path

$$\dot{v} = -\frac{G}{g}. \tag{6}$$

Introducing the mapping

$$y \to v(t, y): \; y = \int_{-\infty}^{v(t, y)} g(t, v')\, \mathrm{d}v',$$

we find

$$1 = \frac{\partial v}{\partial y}(t, y) \cdot g(t, v),$$

and we can perform a difference approximation of $1/g^n$ by

$$\tfrac{1}{2}N(v_{i+1}^n - v_{i-1}^n),$$

where a finite definition of v_0^n and v_{N+1}^n is required. Then we use a simple Euler scheme for the approximation of (6) for the initial values given by the initial-point approximation. This method was tested by Russo [9]. He obtains good results with 40 points.

A hint, why the three ways of the computation of μ_N^{n+1} do not give the same result, is maybe the following. The first method can be described roughly as follows:

$$N_C^{n+1} := \Delta t \int P(k, k')\tilde{\mu}_N^{n+1}(\mathrm{d}k')$$

is the number of points to approximate the gain term. For simplicity we assume $N_C^{n+1} \in \mathbb{N}$. Now, from the points defining $\tilde{\mu}_N^{n+1}$ we keep $N - N_C^{n+1}$ points unchanged and only N_C^{n+1} points get new coordinates according to the gain term. In both other methods all particles can change the coordinates from time step to time step. This shows that we have to investigate the approximation of mixed measures (partially absolutely continuous, partially discrete) by discrete ones. The number-theoretical approach is strong enough for theoretical results but for real algorithms certain additional techniques are necessary.

References

[1] O. Buneman, A giant 3D-code, in: *Proc. Xth Conf. on Numerical Simulation in Plasma Physics*, San Diego, 1982.

[2] M.S. Mock, *Analysis of Mathematical Models of Semi-Conductor Devices* (Boole, Dublin, 1983).

[3] H. Moock, Private communication.

[4] S. Motta, G. Russo, H. Moock and J. Wick, A number-theoretical convergence proof of a point approximation of a space homogeneous transport equation, *Matematiche (Catania)* **41** (1986) 161–178.

[5] K. Nanbu, Stochastic solution method of the master equation and the model Boltzmann equation, *J. Phys. Soc. Japan* **52** (1983) 2654–2658.

[6] H. Neunzert and K.H. Petry, Ein Existenzsatz für die Vlasov-Gleichung mit selbst-konsistentem Magnetfeld, *Math. Methods Appl. Sci.* **2** (1980) 429–444.

[7] H. Neunzert and J. Wick, Die Theorie der asymptotischen Verteilung und die numerische Lösung von Integro-Differentialgleichungen, *Numer. Math.* **21** (1973) 234–243.

[8] L. Reggiani, *Hot-Electron Transport in Semi-Conductors*, Topics Appl. Phys. **58** (Springer, Berlin, 1985).

[9] G. Russo, Private communication.